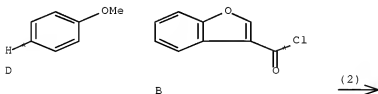
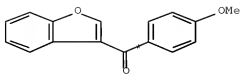


ACCESSION NUMBER: 108:21130 CASREACT Full-text  
 TITLE: Conformational analysis of organic carbonyl  
 compounds.  
 naphthalene  
 AUTHOR(S): Benassi, Rois; Folli, Ugo; Larossi, Dario;  
 Schenetti,  
 Luisa; Taddei, Ferdinando  
 CORPORATE SOURCE: Dip. Chim., Univ. Modena, Modena, 41100, Italy  
 SOURCE: Journal of the Chemical Society, Perkin  
 Transactions  
 2: Physical Organic Chemistry (1972-1999)  
 (1987),  
 (3), 351-7  
 CODEN: JCPKBH; ISSN: 0300-9580  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The conformational anal. of 2- and 3-(p-methoxybenzoyl)benzo[b]furan and -benzo[b]thiophene and 1- and 2-(p-methoxybenzoyl)naphthalene was performed by the NMR lanthanide-induced shift method on <sup>1</sup>H and <sup>13</sup>C chemical shifts with Yb(fod)<sub>3</sub>. In the 2-substituted benzo[b]furan a chelate structure having the lanthanide atom bound to both carbonyl and furyl oxygens is formed, so the results do not represent useful information for the conformational properties of the mol. in solution For the 2-benzo[b]thiophene derivative the S,O-cis (Z) conformation was found to be more abundant in the equilibrium mixture of the two nearly planar conformers. In the corresponding 3-substituted heterocycles the predominant conformation is that of X,O-trans type with a similar degree of distortion from planarity in the two compds. In all these mols. the p-methoxyphenyl ring is twisted .apprx.30° from the carbonyl plane.

RX(2) OF 4 ...D + E ==> E

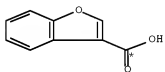




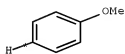
E  
YIELD 44%

RX(2)      RCT D 100-66-3, B 111964-21-7  
             RGT F 7446-70-0 AlCl3  
             PRO E 28222-80-2  
             SOL 75-15-0 CS2

RX(4) OF 4 COMPOSED OF RX(1), RX(2)  
 RX(4)      A + D ==> E

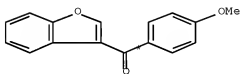


A



D

2  
STEPS  
→



E  
YIELD 44%